FIRST PRINCIPLES CALCULATION OF ENERGY LEVELS AND SPECTRA FOR AB_4, ABC_3 TYPE MOLECULES

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Molecules of type of AB_4 ,ABC_3 are interesting both for experimental and theoretical spectroscopy and for intramolecular dynamics. The spectra of ABC_3 molecules could be calculated on a similar manner as AB_4 molecules (like methane [1] [2]) but specific for these molecules problems have appeared. A big number of PES and DMS parameters requires a much larger number of *ab initio* points for a robust PES and DMS fit. The big number of parameters could also lead to non-physical behaviour of PES far from equilibrium geometry in the 9D space. A full account of the symmetry properties [3] involve smaller dimensions of basis sets and is benefic for handling strict degeneracies and selection rules, particularly in case of transitions among highly excited vibration-rotation states and high temperatures spectra. Full symmetry variational calculations of vibration-rotation energy levels of symmetric five-atomic molecules CH_3Li, CH_3F ([4] [5]), CH_3Cl [6], CH_3Br, CH_4 from a PES are discussed. This work is supported by French-Russian LIA SAMIA. B.M. KRISHNA thanks the Tomsk State University and Academic D.I. Mendeleev Fund Program.

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